Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2026 – 05:35 AM UTC

PDB ID	:	6QS1 / pdb_00006qs1
Title	:	Crystal structure of human Angiotensin-1 converting enzyme N-domain in complex with BPPb
Authors	:	Cozier, G.E.; Acharya, K.R.
Deposited on	:	2019-02-20
Resolution	:	1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

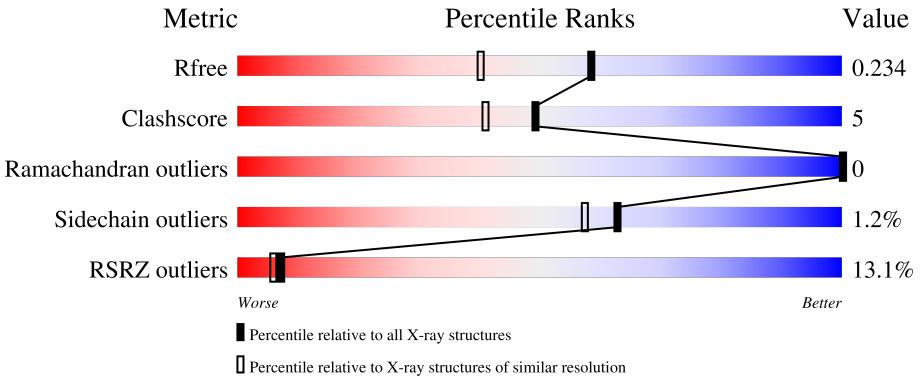
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	629	5% 86% 10% ·
1	B	629	20% 83% 13% ·
2	E	11	36% 64% 27% 9%
2	F	11	36% 9% 55%
3	C	2	50% 50%

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Mol	Chain	Length	Quality of chain
4	D	4	50% 50%
5	G	3	33% 33% 33%
5	H	3	100%
6	I	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	PEG	B	709	-	-	X	-

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 21210 atoms, of which 10081 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	608	Total	C	H	N	O	S	0	19	0
			9851	3230	4811	863	928	19			
1	B	603	Total	C	H	N	O	S	0	17	0
			9776	3203	4785	858	911	19			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	engineered mutation	UNP P12821
A	25	GLN	ASN	engineered mutation	UNP P12821
A	82	GLN	ASN	engineered mutation	UNP P12821
A	117	GLN	ASN	engineered mutation	UNP P12821
A	131	GLN	ASN	engineered mutation	UNP P12821
A	289	GLN	ASN	engineered mutation	UNP P12821
A	545	ARG	GLN	engineered mutation	UNP P12821
A	576	LEU	PRO	engineered mutation	UNP P12821
A	629	LEU	-	expression tag	UNP P12821
B	9	GLN	ASN	engineered mutation	UNP P12821
B	25	GLN	ASN	engineered mutation	UNP P12821
B	82	GLN	ASN	engineered mutation	UNP P12821
B	117	GLN	ASN	engineered mutation	UNP P12821
B	131	GLN	ASN	engineered mutation	UNP P12821
B	289	GLN	ASN	engineered mutation	UNP P12821
B	545	ARG	GLN	engineered mutation	UNP P12821
B	576	LEU	PRO	engineered mutation	UNP P12821
B	629	LEU	-	expression tag	UNP P12821

- Molecule 2 is a protein called Bradykinin potentiating peptide b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	11	Total	C	H	N	O	0	0	0
			176	56	92	15	13			

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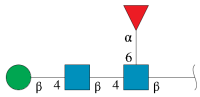
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	5	Total	C	H	N	O	0	0	0
			84	27	45	6	6			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

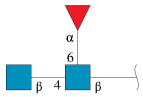
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	4	Total	C	H	N	O	0	0	0
			95	28	46	2	19			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

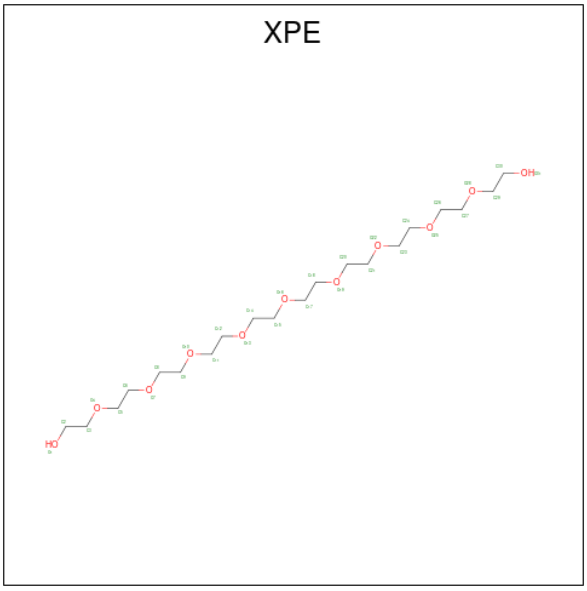


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	3	Total	C	H	N	O	0	0	0
			73	22	35	2	14			
5	H	3	Total	C	H	N	O	0	0	0
			74	22	36	2	14			

- Molecule 6 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

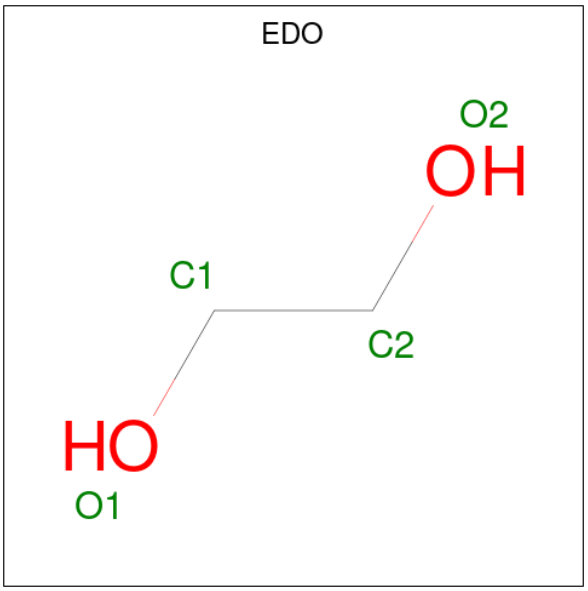
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	I	2	Total	C	H	N	O	0	0	0
			47	14	23	1	9			

- Molecule 7 is 3,6,9,12,15,18,21,24,27-NONAOXANONACOSANE-1,29-DIOL (CCD ID: XPE) (formula: $C_{20}H_{42}O_{11}$).



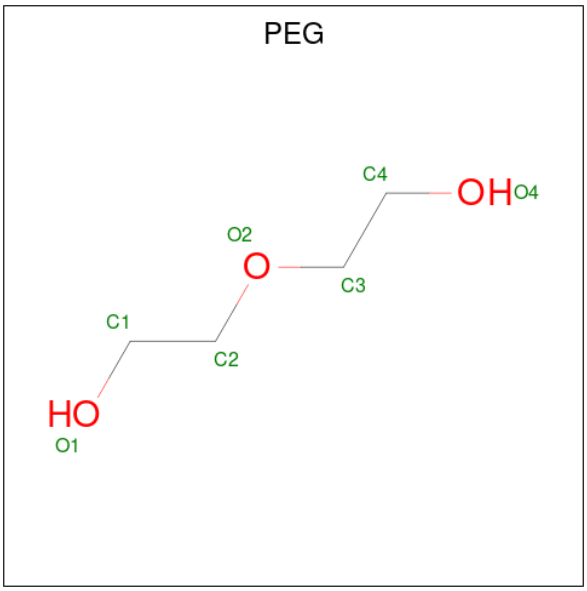
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			73	20	42	11		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



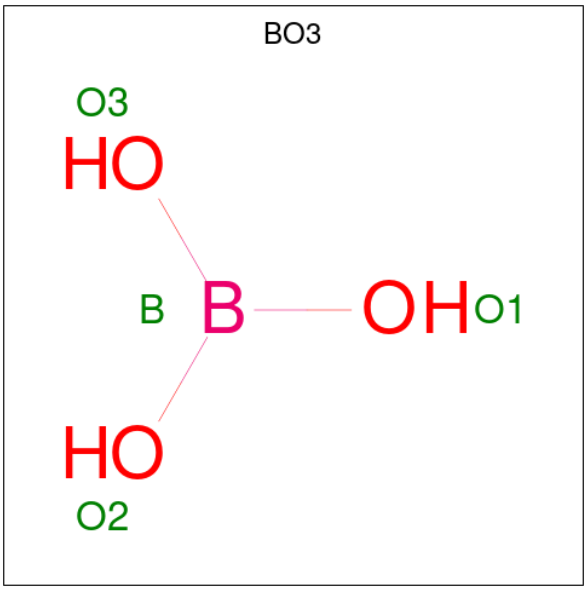
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			10	2	6	2		
8	A	1	Total	C	H	O	0	0
			10	2	6	2		
8	A	1	Total	C	H	O	0	0
			10	2	6	2		
8	A	1	Total	C	H	O	0	0
			10	2	6	2		
8	B	1	Total	C	H	O	0	0
			10	2	6	2		
8	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



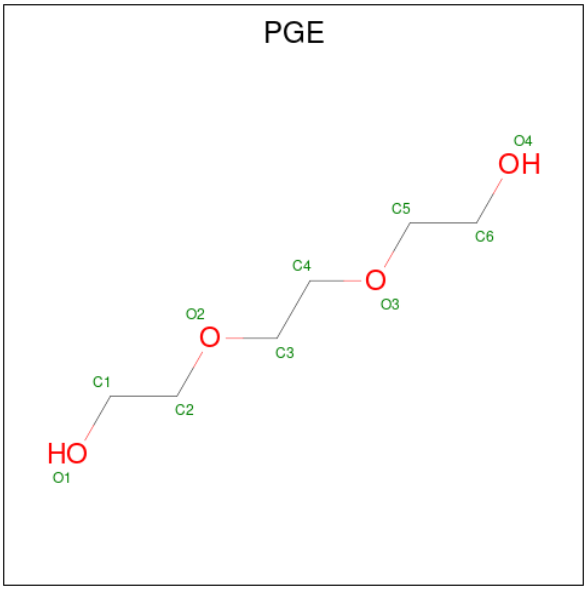
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	0	0
			17	4	10	3		
9	A	1	Total	C	H	O	0	0
			17	4	10	3		
9	B	1	Total	C	H	O	0	0
			17	4	10	3		
9	B	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 10 is BORIC ACID (CCD ID: BO3) (formula: BH_3O_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total B H O 7 1 3 3	0	0
10	A	1	Total B H O 7 1 3 3	0	0
10	A	1	Total B H O 7 1 3 3	0	0
10	A	1	Total B H O 7 1 3 3	0	0
10	B	1	Total B H O 7 1 3 3	0	0
10	B	1	Total B H O 7 1 3 3	0	0
10	B	1	Total B H O 7 1 3 3	0	0

- Molecule 11 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C H O 48 12 28 8	0	1

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total Zn 1 1	0	0
12	B	1	Total Zn 1 1	0	0

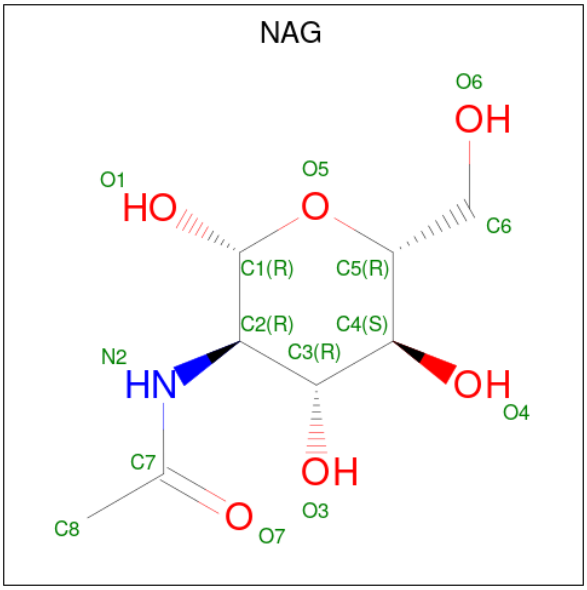
- Molecule 13 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	2	Total Cl 2 2	0	0
13	B	2	Total Cl 2 2	0	0

- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	1	Total Mg 1 1	0	0
14	B	1	Total Mg 1 1	0	0

- Molecule 15 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	B	1	Total C H N O 28 8 14 1 5	0	0

- Molecule 16 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	387	Total O 390 390	0	3

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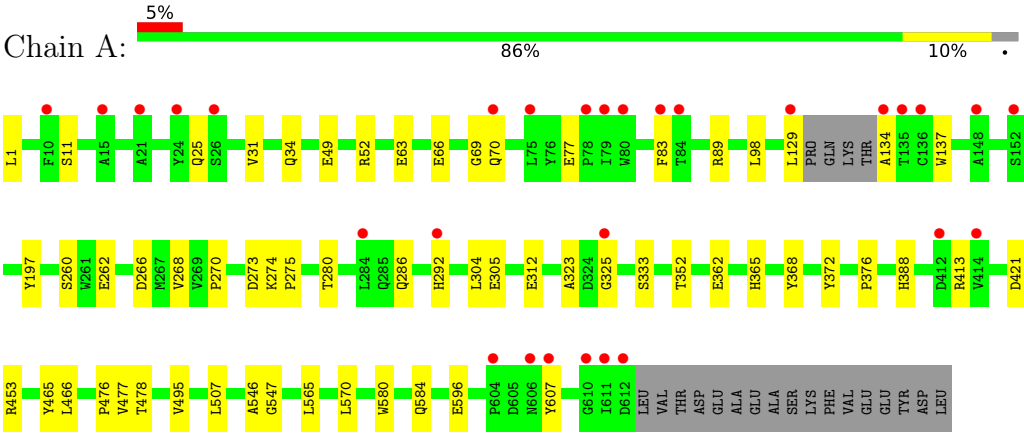
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	B	243	Total O 245 245	0	2
16	E	6	Total O 6 6	0	0
16	F	4	Total O 4 4	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

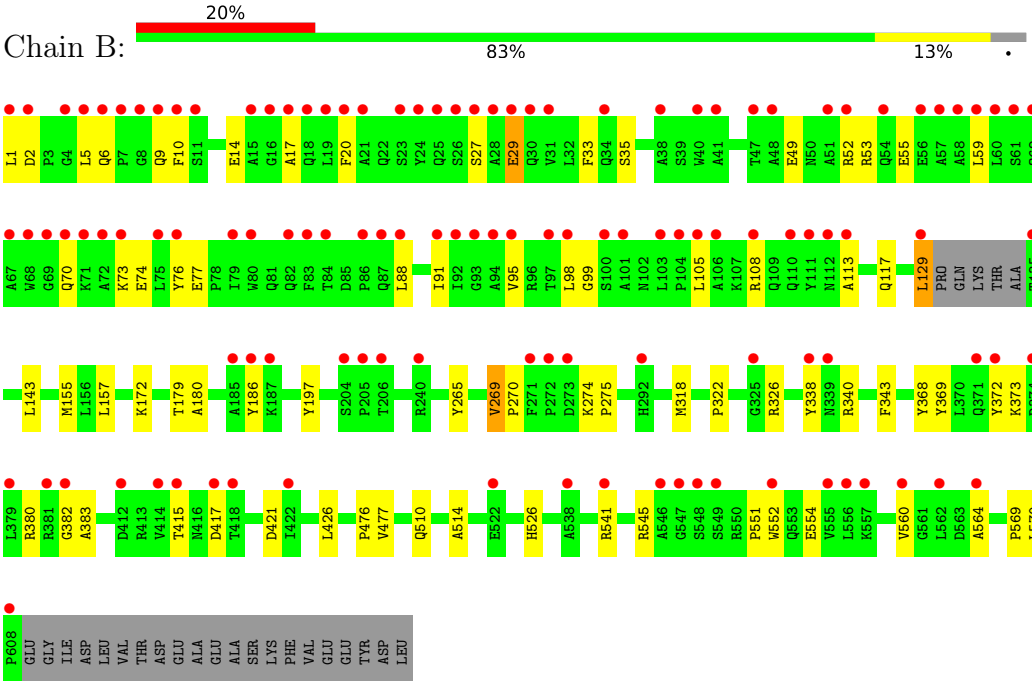
• Molecule 1: Angiotensin-converting enzyme

Chain A:



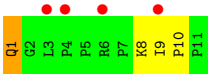
• Molecule 1: Angiotensin-converting enzyme

Chain B:



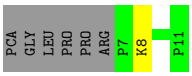
• Molecule 2: Bradykinin potentiating peptide b

Chain E:



• Molecule 2: Bradykinin potentiating peptide b

Chain F:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

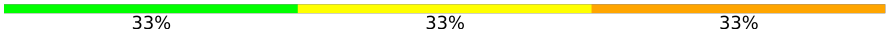
Chain C:

• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

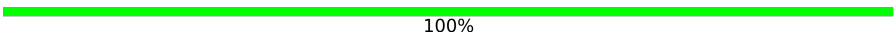
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



• Molecule 6: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	72.68Å 77.07Å 82.36Å 88.86° 64.59° 75.03°	Depositor
Resolution (Å)	74.05 – 1.80 74.05 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (74.05-1.80) 98.6 (74.05-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 1.80Å)	Xtriage
Refinement program	PHENIX (dev_3409: ???)	Depositor
R, R_{free}	0.202 , 0.232 0.203 , 0.234	Depositor DCC
R_{free} test set	1820 reflections (1.16%)	wwPDB-VP
Wilson B-factor (Å^2)	29.8	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 41.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	21210	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XPE, BMA, NAG, EDO, ZN, PGE, PCA, FUC, MG, CL, BO3, PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.53	0/5271	0.66	0/7178
1	B	0.49	0/5220	0.63	0/7109
2	E	0.57	0/81	0.69	0/112
2	F	0.71	0/41	0.66	0/54
All	All	0.51	0/10613	0.65	0/14453

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5040	4811	4741	47	0
1	B	4991	4785	4710	57	0
2	E	84	92	92	4	0
2	F	39	45	45	1	0
3	C	28	27	25	0	0
4	D	49	46	43	0	0
5	G	38	35	34	1	0
5	H	38	36	34	0	0
6	I	24	23	22	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	31	42	42	3	0
8	A	16	24	24	1	0
8	B	8	12	12	0	0
9	A	14	20	20	0	0
9	B	14	20	20	6	0
10	A	16	12	12	0	0
10	B	12	9	9	1	0
11	A	20	28	28	4	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
13	A	2	0	0	0	0
13	B	2	0	0	1	0
14	A	1	0	0	0	0
14	B	1	0	0	0	0
15	B	14	14	13	0	0
16	A	390	0	0	9	0
16	B	245	0	0	7	0
16	E	6	0	0	0	0
16	F	4	0	0	0	0
All	All	11129	10081	9926	111	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (111) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:ALA:HB1	9:B:709:PEG:H42	1.62	0.82
1:A:66:GLU:OE2	16:A:801:HOH:O	1.99	0.79
1:A:157:LEU:HD11	1:A:477:VAL:HG13	1.66	0.77
10:B:712:BO3:O2	16:B:801:HOH:O	2.00	0.77
1:B:377:VAL:HA	1:B:380:ARG:HG3	1.71	0.72
1:B:91:ILE:O	1:B:95:VAL:HG23	1.87	0.72
1:B:375:LEU:O	1:B:380:ARG:NH2	2.25	0.70
1:B:55:GLU:OE2	16:B:803:HOH:O	2.12	0.67
1:A:478:THR:HB	5:G:3:FUC:H61	1.79	0.65
1:A:421:ASP:OD2	16:A:802:HOH:O	2.15	0.64
1:A:25:GLN:OE1	1:A:376:PRO:HA	1.99	0.63
1:B:27:SER:OG	16:B:802:HOH:O	2.10	0.63
1:B:157:LEU:HD11	1:B:477:VAL:HG13	1.79	0.63
1:B:541:ARG:O	1:B:545:ARG:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LEU:HA	1:B:91:ILE:HD12	1.83	0.60
1:A:157:LEU:HD13	1:A:476:PRO:HB2	1.84	0.58
1:A:333:SER:HB3	2:E:9:ILE:HG22	1.85	0.58
1:B:14:GLU:OE2	16:B:805:HOH:O	2.17	0.57
1:A:49:GLU:OE1	1:A:52:ARG:NH2	2.36	0.57
1:B:74:GLU:OE2	16:B:806:HOH:O	2.18	0.56
1:A:495:VAL:HG12	1:A:495:VAL:O	2.07	0.55
1:B:155:MET:HE3	1:B:155:MET:HA	1.87	0.55
1:A:268:VAL:HG21	1:A:430:LEU:HD11	1.90	0.54
1:B:95:VAL:O	16:B:804:HOH:O	2.17	0.54
1:B:186:TYR:CE1	1:B:197:TYR:CE2	2.96	0.54
6:I:1:NAG:O5	6:I:2:FUC:O2	2.21	0.54
1:A:137:TRP:CH2	1:A:155:MET:HE1	2.44	0.53
1:B:59:LEU:O	1:B:63:GLU:HG3	2.09	0.53
1:B:514:ALA:HB2	1:B:560:VAL:HG12	1.92	0.52
1:B:1:LEU:HG	1:B:2:ASP:H	1.75	0.51
1:A:260[B]:SER:HB3	1:A:262[B]:GLU:OE2	2.11	0.51
1:A:466:LEU:HD11	11:A:720[A]:PGE:H12	1.93	0.51
1:A:596:GLU:OE2	6:I:1:NAG:O7	2.28	0.51
1:B:10:PHE:CE2	1:B:20:PHE:HA	2.47	0.49
1:B:265:TYR:CZ	1:B:269:VAL:HG13	2.47	0.49
1:A:362:GLU:OE2	2:E:10:PRO:HD3	2.13	0.49
1:B:274:LYS:NZ	1:B:417:ASP:OD2	2.45	0.49
1:A:266:ASP:OD1	16:A:803:HOH:O	2.20	0.48
1:B:426:LEU:C	1:B:426:LEU:HD13	2.38	0.48
1:A:158:PHE:HA	1:A:607:TYR:OH	2.13	0.48
1:B:180:ALA:HA	9:B:708:PEG:H41	1.96	0.48
1:A:1:LEU:N	1:A:63:GLU:OE1	2.43	0.47
1:A:280:THR:HG23	1:A:352:THR:HA	1.96	0.47
1:A:453:ARG:NH2	16:A:825:HOH:O	2.47	0.47
1:A:270:PRO:HB3	1:A:580:TRP:CH2	2.49	0.47
1:A:413:ARG:NH2	16:A:815:HOH:O	2.35	0.47
1:A:580:TRP:O	1:A:584:GLN:HG2	2.14	0.47
1:B:157:LEU:HD13	1:B:476:PRO:HB2	1.97	0.47
1:B:564:ALA:CB	9:B:709:PEG:H42	2.38	0.47
1:A:274:LYS:HB3	1:A:275:PRO:HD2	1.96	0.47
1:A:69:GLY:HA3	1:A:98:LEU:HD11	1.97	0.47
1:A:197:TYR:OH	2:E:1:PCA:HG3	2.15	0.46
1:B:66:GLU:HG2	1:B:70:GLN:OE1	2.15	0.46
1:A:451:SER:OG	1:A:453:ARG:HG2	2.16	0.46
1:A:365:HIS:CE1	2:E:8:LYS:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:GLU:HG3	1:B:338:TYR:O	2.16	0.46
11:A:720[A]:PGE:C1	16:A:837:HOH:O	2.64	0.46
1:A:137:TRP:HH2	1:A:155:MET:HE1	1.81	0.45
1:A:570:LEU:C	1:A:570:LEU:HD23	2.40	0.45
11:A:720[A]:PGE:H1	16:A:837:HOH:O	2.15	0.45
1:B:510:GLN:HG2	1:B:569:PRO:HG2	1.98	0.45
1:A:274:LYS:HB3	1:A:275:PRO:CD	2.47	0.45
1:B:564:ALA:HB1	9:B:709:PEG:C4	2.41	0.45
13:B:716:CL:CL	2:F:8:LYS:NZ	2.81	0.44
1:B:99:GLY:HA2	1:B:186:TYR:CE1	2.52	0.44
1:B:139:LEU:HA	1:B:143:LEU:HD12	1.98	0.44
1:B:73:LYS:HA	1:B:77:GLU:HB2	1.99	0.44
1:A:507:LEU:HD13	1:A:565:LEU:CD2	2.48	0.44
1:B:552:TRP:HH2	9:B:709:PEG:O4	2.00	0.44
1:A:323:ALA:C	1:A:325:GLY:H	2.26	0.43
8:A:718:EDO:H11	16:A:828:HOH:O	2.17	0.43
1:B:9:GLN:C	1:B:10:PHE:CD1	2.96	0.43
1:B:186:TYR:CE1	1:B:197:TYR:CD2	3.06	0.43
1:B:17:ALA:HB2	1:B:76:TYR:CE1	2.52	0.43
1:A:129:LEU:HD21	1:A:134:ALA:CB	2.49	0.43
1:A:286:GLN:O	7:A:710:XPE:H151	2.19	0.43
1:B:73:LYS:O	1:B:77:GLU:HB2	2.18	0.43
1:A:129:LEU:HD21	1:A:134:ALA:HB2	2.00	0.43
1:A:31:VAL:O	1:A:34:GLN:HG3	2.19	0.43
1:B:274:LYS:HB3	1:B:275:PRO:CD	2.49	0.43
1:B:77:GLU:HA	1:B:77:GLU:OE1	2.19	0.43
1:B:382:GLY:O	1:B:383:ALA:C	2.61	0.43
1:B:318:MET:HE3	1:B:322:PRO:HD3	2.00	0.42
1:A:312:GLU:OE1	1:A:312:GLU:N	2.39	0.42
1:A:66:GLU:O	1:A:70:GLN:HG3	2.19	0.42
1:A:292:HIS:NE2	7:A:710:XPE:C17	2.83	0.42
1:A:292:HIS:NE2	7:A:710:XPE:H172	2.33	0.42
1:B:2:ASP:O	1:B:6:GLN:HG3	2.19	0.42
1:B:49:GLU:O	1:B:53:ARG:HG3	2.19	0.42
1:B:551:PRO:HG2	1:B:554:GLU:CD	2.44	0.42
1:B:129:LEU:HD21	1:B:137:TRP:CH2	2.55	0.42
1:B:179:THR:HG22	9:B:708:PEG:H32	2.00	0.42
1:B:105:LEU:HA	1:B:108:ARG:HD2	2.02	0.42
1:B:172:LYS:NZ	16:B:808:HOH:O	2.24	0.42
1:A:83:PHE:HB2	1:A:89:ARG:HG2	2.00	0.42
1:B:113:ALA:O	1:B:117:GLN:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:LEU:HD23	1:B:27:SER:HB3	2.03	0.41
1:A:507:LEU:HD13	1:A:565:LEU:HD23	2.02	0.41
1:A:465:TYR:CE2	11:A:720[A]:PGE:H32	2.56	0.41
1:B:421:ASP:CG	1:B:526:HIS:HE2	2.29	0.41
1:B:33:PHE:CD1	1:B:33:PHE:C	2.98	0.41
1:B:52:ARG:HH12	1:B:53:ARG:HH12	1.69	0.41
1:A:77:GLU:HA	1:A:77:GLU:OE1	2.21	0.41
1:A:546:ALA:O	1:A:547:GLY:C	2.62	0.41
1:B:570:LEU:HD23	1:B:570:LEU:C	2.46	0.41
1:B:340:ARG:HG2	1:B:373:LYS:O	2.22	0.40
1:B:343:PHE:CE2	1:B:369:TYR:HB3	2.56	0.40
1:A:304:LEU:O	1:A:305:GLU:HB2	2.21	0.40
1:B:270:PRO:HB3	1:B:580:TRP:CH2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	623/629 (99%)	611 (98%)	12 (2%)	0	100	100
1	B	616/629 (98%)	599 (97%)	17 (3%)	0	100	100
2	E	9/11 (82%)	8 (89%)	1 (11%)	0	100	100
2	F	3/11 (27%)	3 (100%)	0	0	100	100
All	All	1251/1280 (98%)	1221 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	540/541 (100%)	535 (99%)	5 (1%)	70 67
1	B	534/541 (99%)	526 (98%)	8 (2%)	57 49
2	E	9/9 (100%)	9 (100%)	0	100 100
2	F	5/9 (56%)	5 (100%)	0	100 100
All	All	1088/1100 (99%)	1075 (99%)	13 (1%)	63 57

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	273	ASP
1	A	368	TYR
1	A	372	TYR
1	A	388	HIS
1	B	29	GLU
1	B	35	SER
1	B	129	LEU
1	B	269	VAL
1	B	326	ARG
1	B	368	TYR
1	B	372	TYR
1	B	415	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	70	GLN
1	A	588	ASN
1	B	18	GLN
1	B	25	GLN
1	B	371	GLN

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Mol	Chain	Res	Type
1	B	606	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PCA	E	1	2	7,8,9	2.57	2 (28%)	9,10,12	2.07	6 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PCA	E	1	2	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	PCA	CD-N	5.18	1.47	1.34
2	E	1	PCA	CA-N	4.20	1.51	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	PCA	CA-N-CD	-3.02	103.24	113.58
2	E	1	PCA	CB-CA-N	2.81	110.97	103.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	PCA	CB-CA-C	-2.45	109.30	112.66
2	E	1	PCA	OE-CD-CG	-2.33	122.56	126.72
2	E	1	PCA	CG-CD-N	2.28	113.98	108.39
2	E	1	PCA	O-C-CA	-2.03	119.54	124.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	PCA	1	0

5.5 Carbohydrates (i)

14 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	C	1	1,3	14,14,15	0.40	0	17,19,21	0.54	0
3	NAG	C	2	3	14,14,15	0.20	0	17,19,21	0.76	1 (5%)
4	NAG	D	1	1,4	14,14,15	0.59	0	17,19,21	0.62	0
4	NAG	D	2	4	14,14,15	0.37	0	17,19,21	0.77	1 (5%)
4	BMA	D	3	4	11,11,12	0.98	0	15,15,17	0.73	0
4	FUC	D	4	4	10,10,11	0.92	1 (10%)	14,14,16	1.14	2 (14%)
5	NAG	G	1	1,5	14,14,15	0.51	0	17,19,21	0.88	1 (5%)
5	NAG	G	2	5	14,14,15	0.48	0	17,19,21	0.48	0
5	FUC	G	3	5	10,10,11	1.04	1 (10%)	14,14,16	1.21	2 (14%)
5	NAG	H	1	1,5	14,14,15	0.44	0	17,19,21	0.54	0
5	NAG	H	2	5	14,14,15	0.45	0	17,19,21	0.44	0
5	FUC	H	3	5	10,10,11	0.72	0	14,14,16	0.90	0
6	NAG	I	1	1,6	14,14,15	0.80	1 (7%)	17,19,21	0.86	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	FUC	I	2	6	10,10,11	0.84	0	14,14,16	1.54	3 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	FUC	D	4	4	-	-	0/1/1/1
5	NAG	G	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	FUC	G	3	5	-	-	0/1/1/1
5	NAG	H	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	FUC	H	3	5	-	-	0/1/1/1
6	NAG	I	1	1,6	-	2/6/23/26	0/1/1/1
6	FUC	I	2	6	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	4	FUC	O5-C1	-2.36	1.39	1.43
5	G	3	FUC	C1-C2	2.23	1.57	1.52
6	I	1	NAG	C1-C2	2.19	1.55	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	2	FUC	C1-C2-C3	3.64	114.94	109.64
6	I	1	NAG	C1-O5-C5	3.06	116.29	112.19
5	G	3	FUC	O2-C2-C1	2.85	115.75	109.22
6	I	2	FUC	C1-O5-C5	2.58	119.05	112.97
5	G	1	NAG	C1-O5-C5	2.24	115.19	112.19
4	D	2	NAG	C1-O5-C5	2.24	115.19	112.19
6	I	2	FUC	O5-C1-C2	2.23	116.11	110.79
3	C	2	NAG	C1-O5-C5	2.18	115.11	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	4	FUC	O3-C3-C4	-2.10	105.44	110.38
4	D	4	FUC	O5-C5-C4	2.02	113.19	109.55
5	G	3	FUC	C1-O5-C5	2.02	117.72	112.97

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	2	NAG	C1-C2-N2-C7
6	I	1	NAG	O5-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
5	G	1	NAG	C3-C2-N2-C7
5	G	1	NAG	C1-C2-N2-C7
5	G	2	NAG	C3-C2-N2-C7

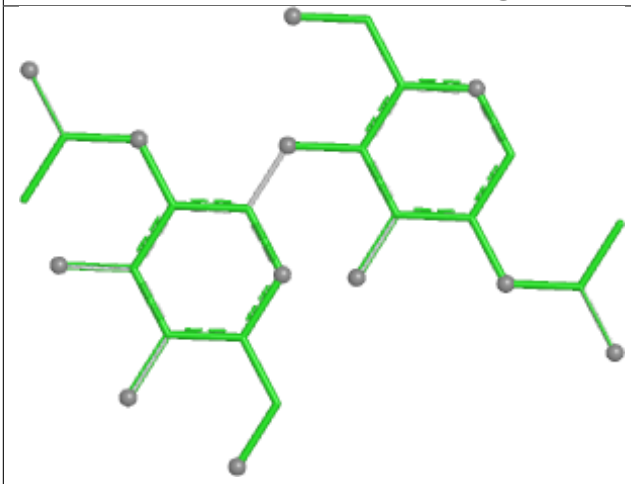
There are no ring outliers.

3 monomers are involved in 3 short contacts:

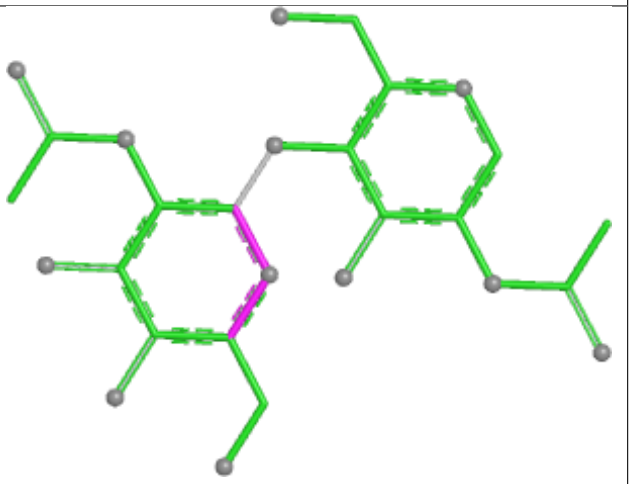
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	2	FUC	1	0
5	G	3	FUC	1	0
6	I	1	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

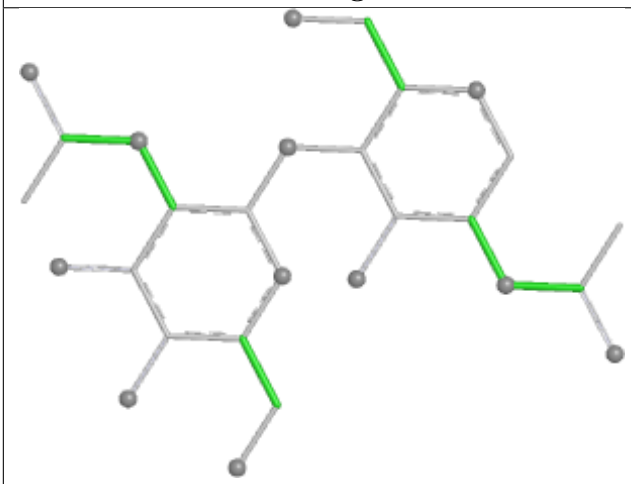
Oligosaccharide Chain C



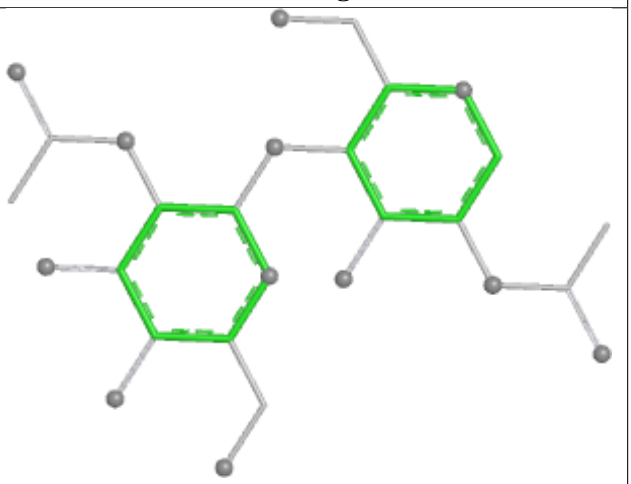
Bond lengths



Bond angles

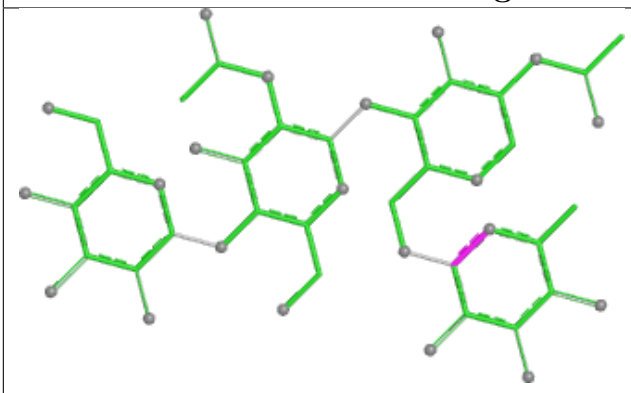


Torsions

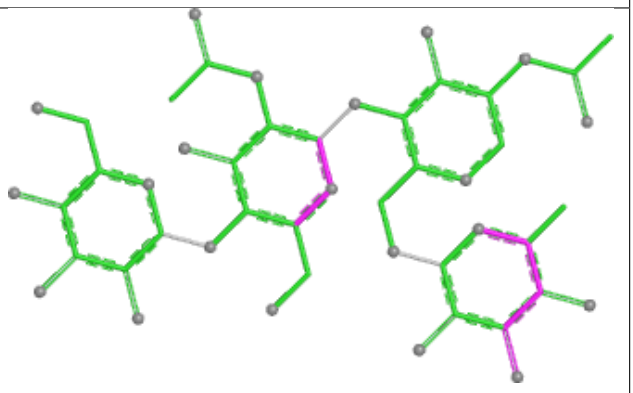


Rings

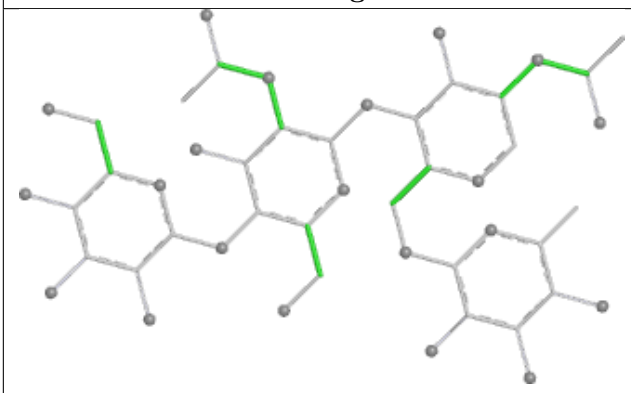
Oligosaccharide Chain D



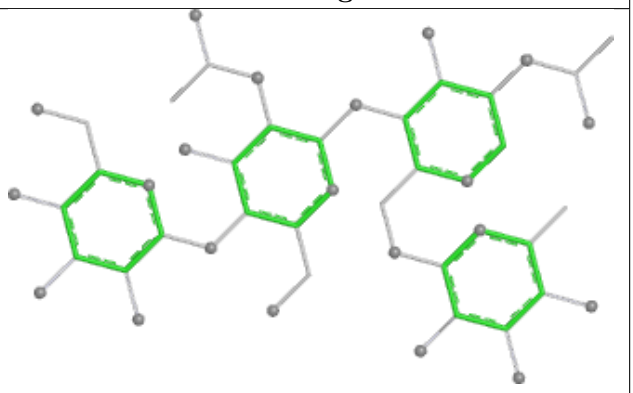
Bond lengths



Bond angles

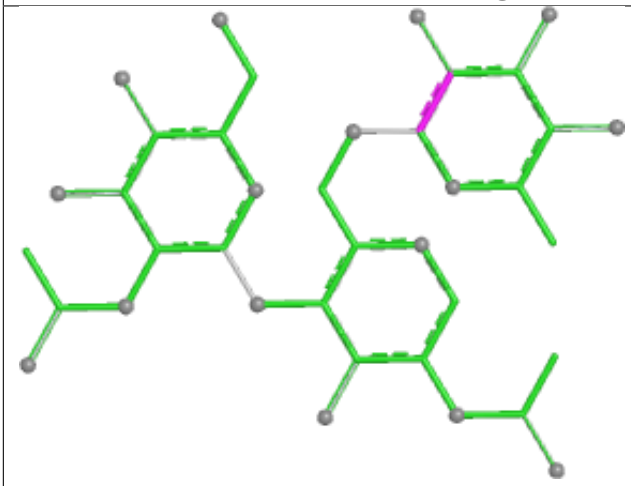


Torsions

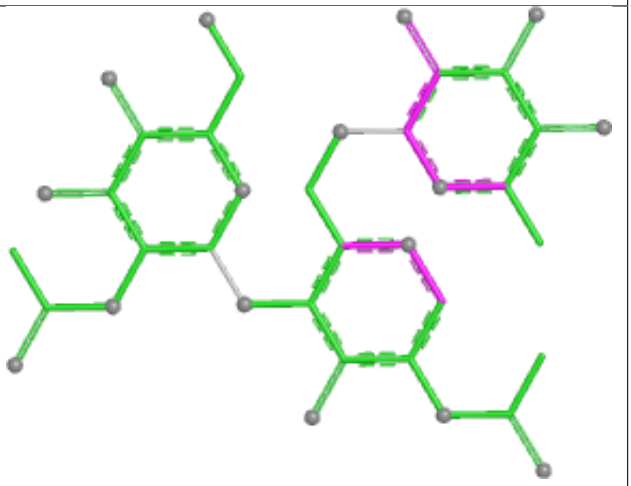


Rings

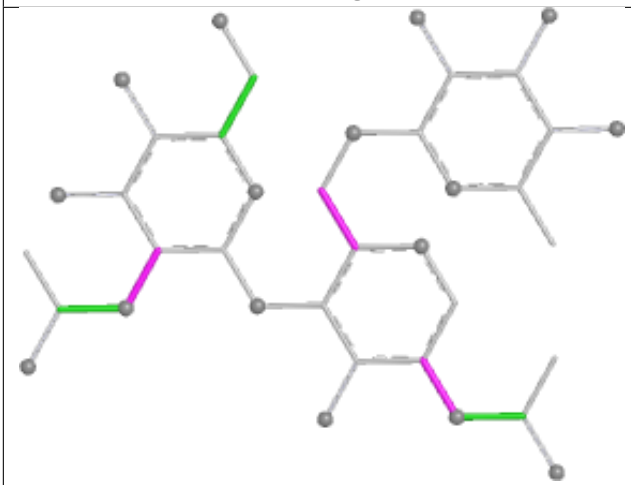
Oligosaccharide Chain G



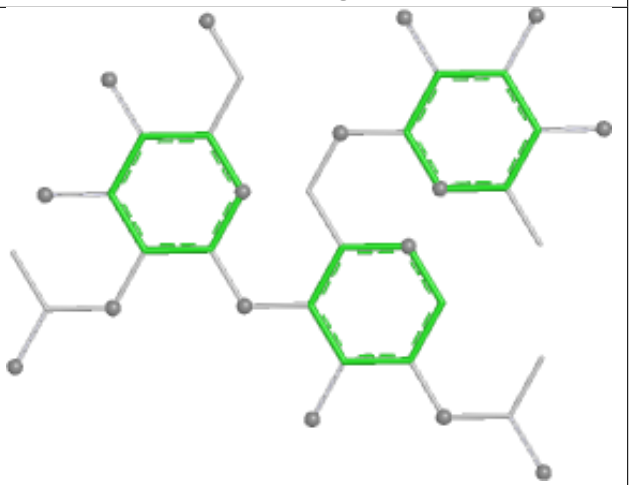
Bond lengths



Bond angles

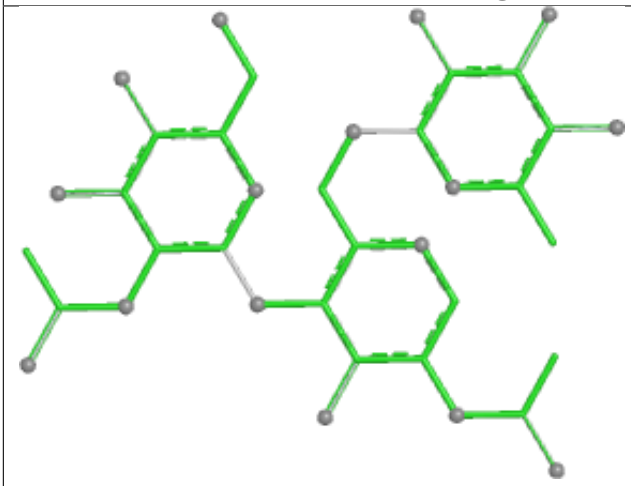


Torsions

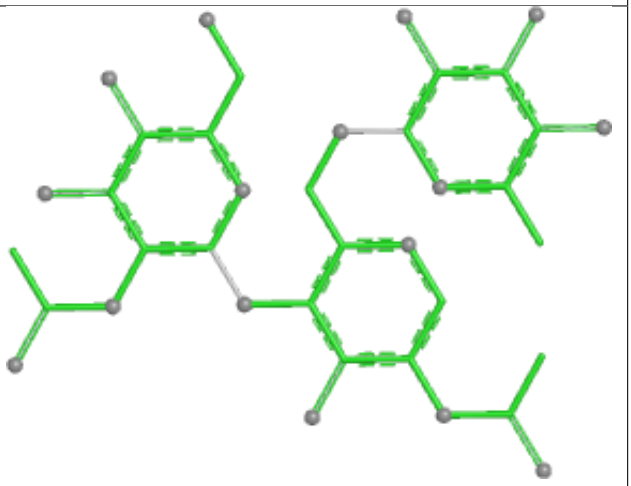


Rings

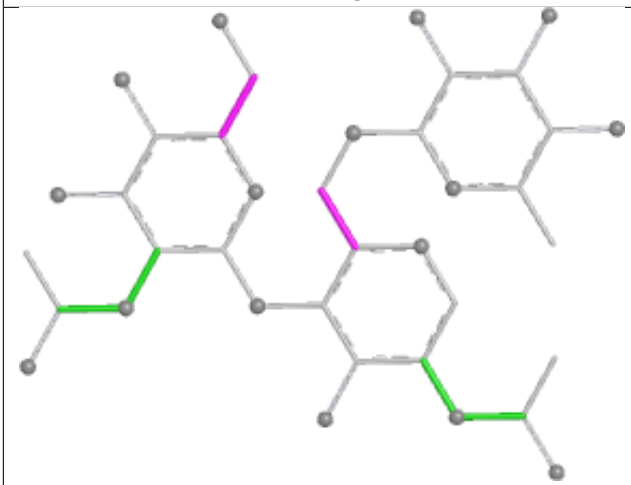
Oligosaccharide Chain H



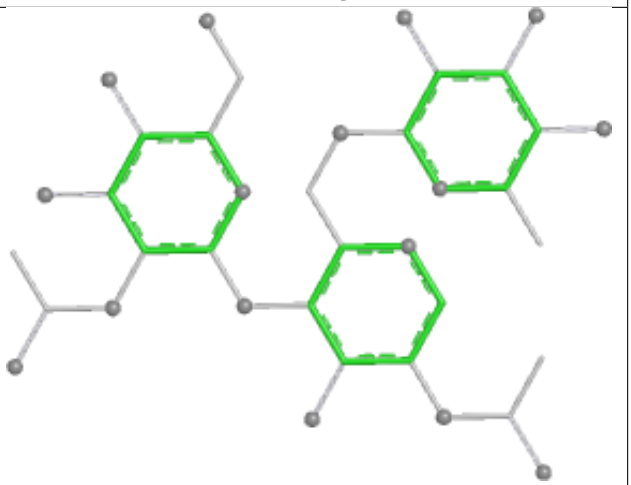
Bond lengths



Bond angles

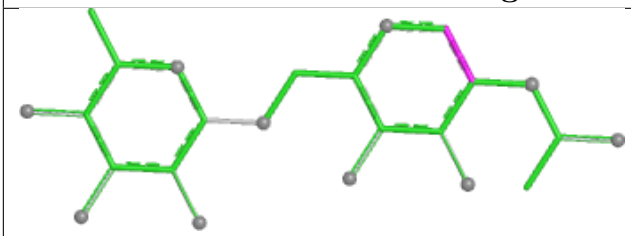


Torsions

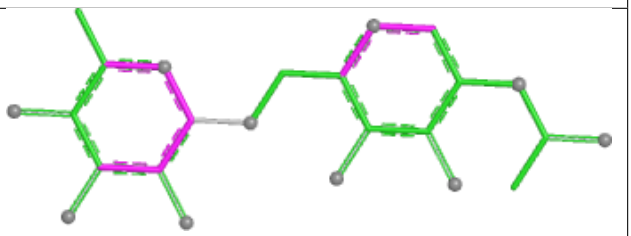


Rings

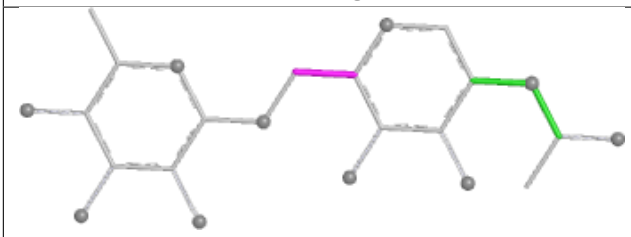
Oligosaccharide Chain I



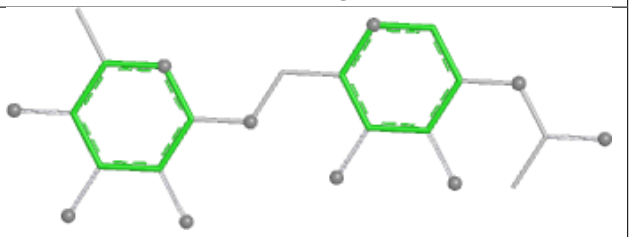
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 29 ligands modelled in this entry, 8 are monoatomic - leaving 21 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	EDO	A	719	-	3,3,3	0.46	0	2,2,2	0.68	0
8	EDO	B	707	-	3,3,3	0.52	0	2,2,2	0.15	0
9	PEG	B	709	-	6,6,6	0.53	0	5,5,5	0.42	0
9	PEG	A	713	-	6,6,6	0.52	0	5,5,5	0.44	0
11	PGE	A	720[A]	-	9,9,9	0.37	0	8,8,8	0.46	0
10	BO3	A	716	-	3,3,3	0.20	0	3,3,3	0.53	0
10	BO3	B	712	-	3,3,3	0.51	0	3,3,3	0.27	0
8	EDO	B	713	-	3,3,3	0.44	0	2,2,2	0.45	0
10	BO3	B	711	-	3,3,3	0.25	0	3,3,3	0.16	0
9	PEG	B	708	-	6,6,6	0.54	0	5,5,5	0.41	0
8	EDO	A	718	-	3,3,3	0.50	0	2,2,2	0.48	0
10	BO3	A	721	-	3,3,3	0.24	0	3,3,3	0.38	0
15	NAG	B	701	1	14,14,15	0.56	0	17,19,21	0.56	0
11	PGE	A	720[B]	-	9,9,9	0.31	0	8,8,8	0.65	0
10	BO3	A	715	-	3,3,3	0.47	0	3,3,3	0.67	0
10	BO3	A	714	-	3,3,3	0.75	0	3,3,3	0.73	0
8	EDO	A	711	-	3,3,3	0.52	0	2,2,2	0.29	0
7	XPE	A	710	-	30,30,30	0.60	0	29,29,29	0.67	0
9	PEG	A	717	-	6,6,6	0.45	0	5,5,5	0.47	0
10	BO3	B	710	-	3,3,3	0.30	0	3,3,3	0.50	0
8	EDO	A	712	-	3,3,3	0.41	0	2,2,2	0.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	B	713	-	-	1/1/1/1	-
11	PGE	A	720[B]	-	-	6/7/7/7	-
15	NAG	B	701	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	A	719	-	-	0/1/1/1	-
8	EDO	A	712	-	-	1/1/1/1	-
8	EDO	B	707	-	-	0/1/1/1	-
9	PEG	B	709	-	-	4/4/4/4	-
9	PEG	B	708	-	-	2/4/4/4	-
8	EDO	A	718	-	-	1/1/1/1	-
9	PEG	A	713	-	-	2/4/4/4	-
8	EDO	A	711	-	-	0/1/1/1	-
7	XPE	A	710	-	-	15/28/28/28	-
11	PGE	A	720[A]	-	-	3/7/7/7	-
9	PEG	A	717	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	720[A]	PGE	O2-C3-C4-O3
7	A	710	XPE	O7-C8-C9-O10
9	B	708	PEG	O1-C1-C2-O2
9	B	709	PEG	O1-C1-C2-O2
11	A	720[B]	PGE	O3-C5-C6-O4
9	B	709	PEG	O2-C3-C4-O4
11	A	720[B]	PGE	O1-C1-C2-O2
9	A	713	PEG	O1-C1-C2-O2
11	A	720[A]	PGE	O1-C1-C2-O2
15	B	701	NAG	C4-C5-C6-O6
8	A	718	EDO	O1-C1-C2-O2
11	A	720[B]	PGE	C1-C2-O2-C3
9	A	717	PEG	O1-C1-C2-O2
9	B	708	PEG	O2-C3-C4-O4
11	A	720[A]	PGE	C6-C5-O3-C4
15	B	701	NAG	O5-C5-C6-O6
15	B	701	NAG	C1-C2-N2-C7
9	B	709	PEG	C1-C2-O2-C3
7	A	710	XPE	C20-C21-O22-C23
7	A	710	XPE	O1-C2-C3-O4
9	A	713	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
9	B	709	PEG	C4-C3-O2-C2
9	A	717	PEG	O2-C3-C4-O4
11	A	720[B]	PGE	C6-C5-O3-C4
7	A	710	XPE	C27-C26-O25-C24
9	A	717	PEG	C1-C2-O2-C3
8	B	713	EDO	O1-C1-C2-O2
15	B	701	NAG	C3-C2-N2-C7
7	A	710	XPE	C23-C24-O25-C26
7	A	710	XPE	O10-C11-C12-O13
7	A	710	XPE	O16-C17-C18-O19
7	A	710	XPE	C14-C15-O16-C17
7	A	710	XPE	O22-C23-C24-O25
7	A	710	XPE	C5-C6-O7-C8
8	A	712	EDO	O1-C1-C2-O2
7	A	710	XPE	O4-C5-C6-O7
7	A	710	XPE	C2-C3-O4-C5
11	A	720[B]	PGE	C4-C3-O2-C2
7	A	710	XPE	C30-C29-O28-C27
7	A	710	XPE	C21-C20-O19-C18
7	A	710	XPE	C24-C23-O22-C21
11	A	720[B]	PGE	O2-C3-C4-O3

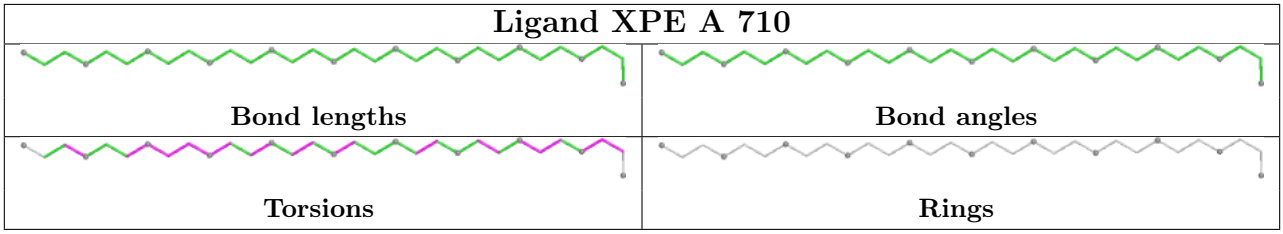
There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	709	PEG	4	0
11	A	720[A]	PGE	4	0
10	B	712	BO3	1	0
9	B	708	PEG	2	0
8	A	718	EDO	1	0
7	A	710	XPE	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	608/629 (96%)	0.28	29 (4%) 35 34	13, 38, 60, 87	10 (1%)
1	B	603/629 (95%)	0.96	127 (21%) 2 2	17, 47, 73, 97	8 (1%)
2	E	10/11 (90%)	2.14	4 (40%) 1 0	24, 39, 49, 49	10 (100%)
2	F	5/11 (45%)	0.72	0 100 100	28, 32, 43, 45	5 (100%)
All	All	1226/1280 (95%)	0.63	160 (13%) 7 6	13, 41, 70, 97	33 (2%)

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	3	LEU	5.8
1	A	325	GLY	5.5
1	B	10	PHE	5.2
1	B	24	TYR	5.1
1	B	64	PHE	5.1
1	A	134	ALA	5.1
1	B	68	TRP	4.9
1	B	92	ILE	4.8
1	A	129	LEU	4.8
1	B	80	TRP	4.6
1	B	375	LEU	4.5
1	B	101[A]	ALA	4.5
1	B	25	GLN	4.3
1	B	271	PHE	4.3
1	B	20	PHE	4.2
1	B	105	LEU	4.2
1	B	1	LEU	4.2
1	B	59	LEU	4.1
1	B	82	GLN	4.0
1	B	5	LEU	4.0
1	A	611	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	21	ALA	4.0
1	B	75	LEU	4.0
1	B	547	GLY	3.9
1	A	607	TYR	3.9
1	B	31	VAL	3.8
1	B	135	THR	3.8
1	B	38	ALA	3.8
1	B	93	GLY	3.6
1	A	135	THR	3.6
1	B	48	ALA	3.5
1	B	418	THR	3.5
1	B	60	LEU	3.5
1	A	136	CYS	3.5
1	B	608	PRO	3.5
1	B	206	THR	3.4
1	B	72	ALA	3.4
1	A	606	ASN	3.4
1	B	272	PRO	3.4
1	A	79	ILE	3.4
1	B	95	VAL	3.4
1	A	414	VAL	3.4
1	B	113	ALA	3.4
1	B	79	ILE	3.3
2	E	9	ILE	3.3
1	B	8	GLY	3.3
1	B	23	SER	3.3
1	B	4	GLY	3.3
1	B	15	ALA	3.2
1	B	28	ALA	3.2
1	B	325	GLY	3.2
1	B	549	SER	3.2
1	B	51	ALA	3.1
1	B	26	SER	3.1
1	B	65	ALA	3.1
1	B	548	SER	3.1
1	B	56	GLU	3.1
1	B	98	LEU	3.1
1	B	91	ILE	3.0
1	B	83	PHE	3.0
1	B	546	ALA	3.0
1	B	129	LEU	3.0
1	A	292	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	17	ALA	3.0
1	B	58	ALA	3.0
1	B	185	ALA	3.0
1	B	7	PRO	2.9
1	A	284	LEU	2.9
1	B	106	ALA	2.9
1	B	541	ARG	2.9
1	B	379	LEU	2.9
1	B	555	VAL	2.8
1	B	9	GLN	2.8
1	B	61[A]	SER	2.8
1	B	88	LEU	2.8
1	B	374	ASP	2.8
1	B	67	ALA	2.8
1	A	80	TRP	2.8
1	B	47	THR	2.8
1	B	27	SER	2.7
1	A	24	TYR	2.7
1	B	57	ALA	2.7
1	A	78	PRO	2.7
1	B	76	TYR	2.7
1	B	86	PRO	2.7
1	B	94	ALA	2.7
1	B	564	ALA	2.7
1	B	562	LEU	2.7
2	E	4	PRO	2.7
1	B	292	HIS	2.7
1	B	2	ASP	2.6
1	B	552	TRP	2.6
1	B	100[A]	SER	2.6
1	B	103	LEU	2.6
1	B	29	GLU	2.6
1	B	97	THR	2.6
1	B	205	PRO	2.6
1	B	69	GLY	2.6
1	B	412	ASP	2.6
1	B	338	TYR	2.6
1	B	372	TYR	2.6
1	B	41	ALA	2.6
1	B	71	LYS	2.5
1	B	34	GLN	2.5
1	B	104	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	148	ALA	2.5
1	A	612	ASP	2.5
1	B	186	TYR	2.4
1	B	377	VAL	2.4
1	B	6	GLN	2.4
1	A	610	GLY	2.4
1	A	21	ALA	2.4
1	B	187	LYS	2.4
1	A	75	LEU	2.3
1	B	54	GLN	2.3
1	B	16	GLY	2.3
1	B	381	ARG	2.3
1	B	136	CYS	2.3
1	B	70	GLN	2.3
1	B	371	GLN	2.3
1	B	111	TYR	2.3
1	B	112	ASN	2.3
1	A	83	PHE	2.3
1	B	73	LYS	2.3
1	A	84	THR	2.3
1	B	11	SER	2.2
1	B	273	ASP	2.2
1	A	26	SER	2.2
1	B	204	SER	2.2
1	A	10	PHE	2.2
1	B	522	GLU	2.2
1	B	84	THR	2.2
1	B	415	THR	2.2
1	B	62[A]	GLN	2.2
1	A	604	PRO	2.2
1	B	557	LYS	2.2
1	B	422	ILE	2.1
1	B	40	TRP	2.1
1	A	412	ASP	2.1
1	B	417	ASP	2.1
1	B	52	ARG	2.1
1	B	607	TYR	2.1
1	B	382	GLY	2.1
2	E	6	ARG	2.1
1	B	19	LEU	2.1
1	B	18	GLN	2.1
1	B	110	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	538	ALA	2.1
1	B	108	ARG	2.1
1	B	339	ASN	2.1
1	B	560	VAL	2.1
1	B	87	GLN	2.1
1	B	556	LEU	2.1
1	B	63	GLU	2.0
1	B	30	GLN	2.0
1	A	15	ALA	2.0
1	A	152	SER	2.0
1	A	70	GLN	2.0
1	B	240	ARG	2.0
1	B	414	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PCA	E	1	8/9	0.84	0.15	45,55,60,65	14

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	C	1	14/15	-	-	49,61,74,78	0
3	NAG	C	2	14/15	-	-	61,81,98,103	0
4	NAG	D	1	14/15	-	-	38,46,58,58	0
4	NAG	D	2	14/15	-	-	46,58,75,75	27
4	BMA	D	3	11/12	-	-	65,76,88,92	0
4	FUC	D	4	10/11	-	-	42,50,60,63	20
6	FUC	I	2	10/11	0.62	0.23	59,71,86,94	20
5	FUC	H	3	10/11	0.65	0.23	64,71,81,83	20
5	NAG	G	2	14/15	0.72	0.18	60,73,93,103	27

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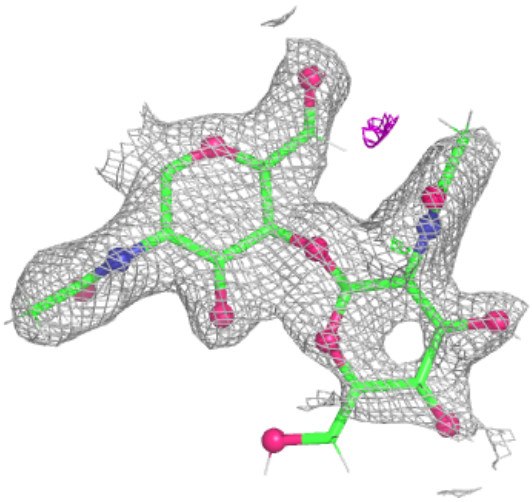
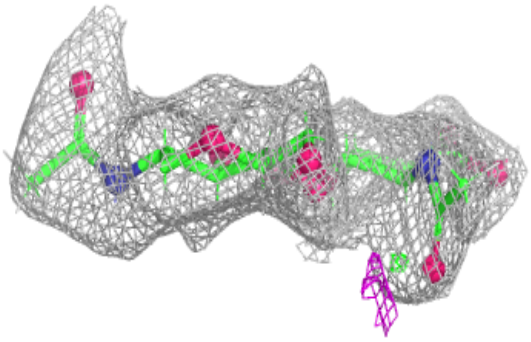
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	FUC	G	3	10/11	0.76	0.16	54,65,82,91	0
5	NAG	H	1	14/15	0.79	0.13	57,67,81,81	0
5	NAG	H	2	14/15	0.79	0.17	62,71,86,86	28
6	NAG	I	1	14/15	0.82	0.14	49,60,74,86	0
5	NAG	G	1	14/15	0.91	0.12	43,55,67,68	0

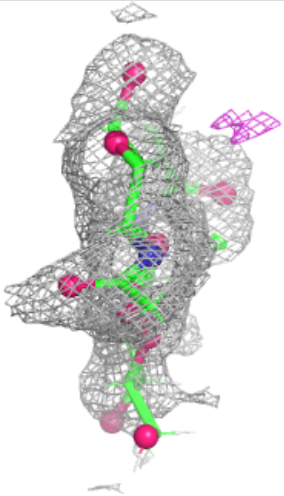
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

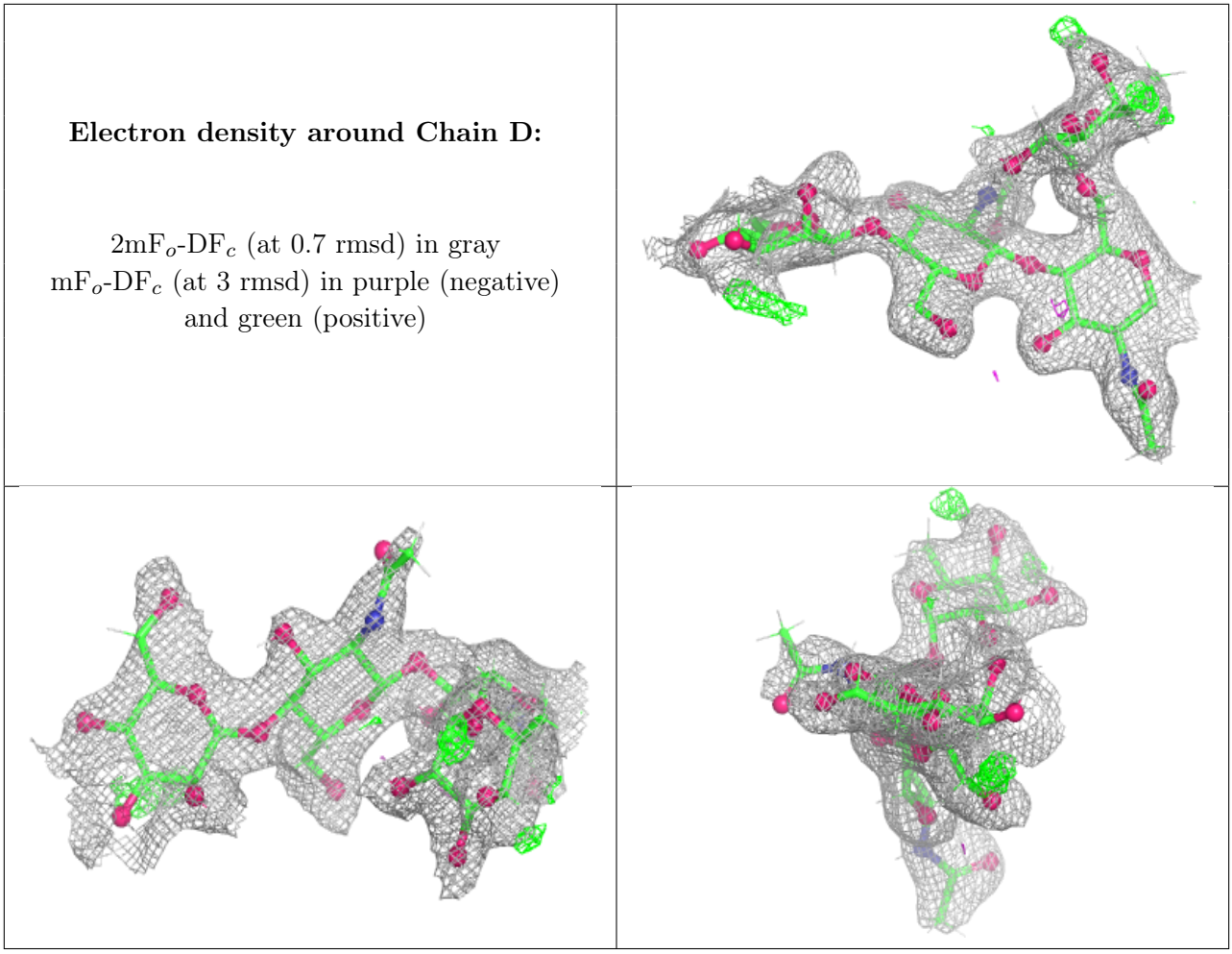






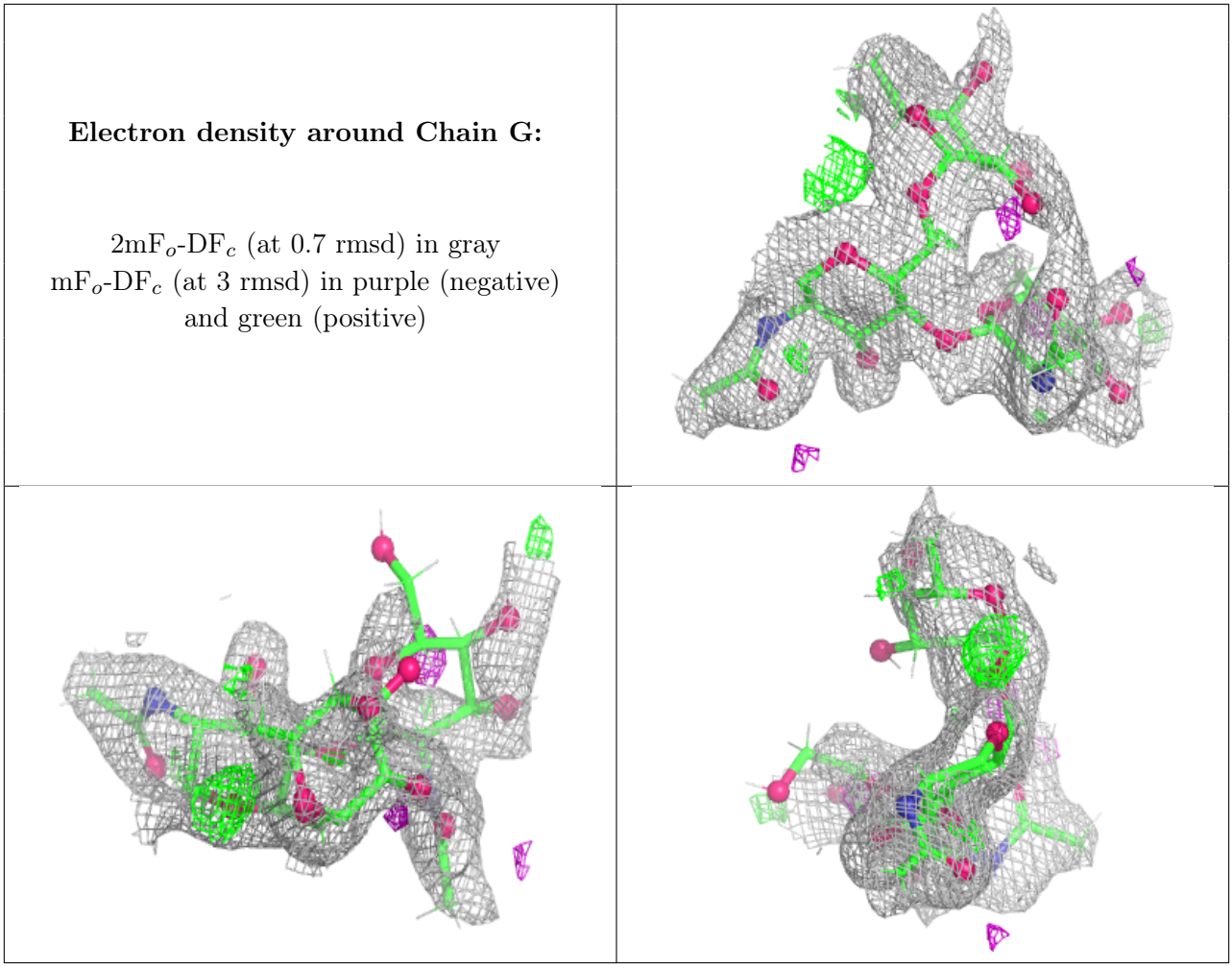
Electron density around Chain D:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



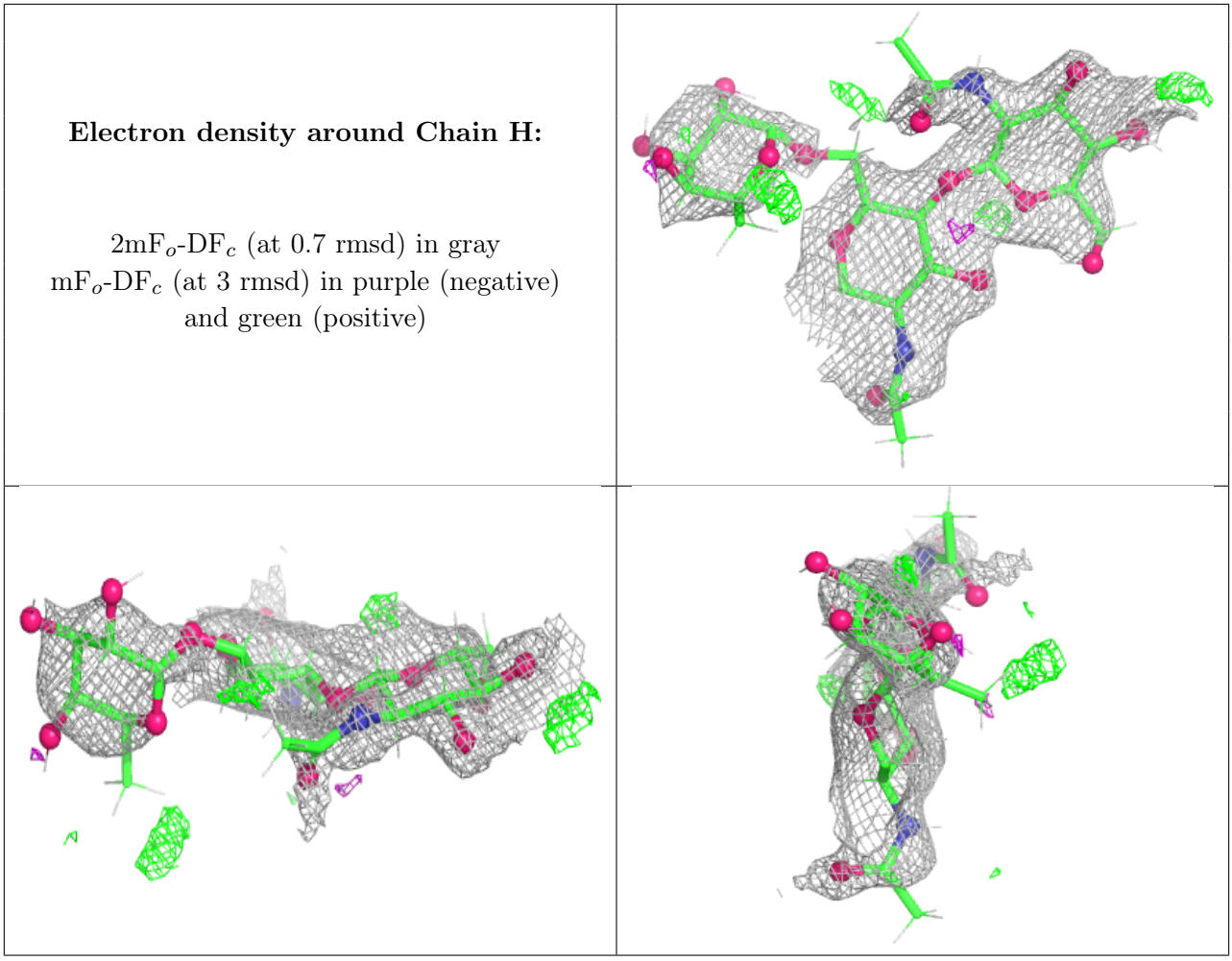
Electron density around Chain G:

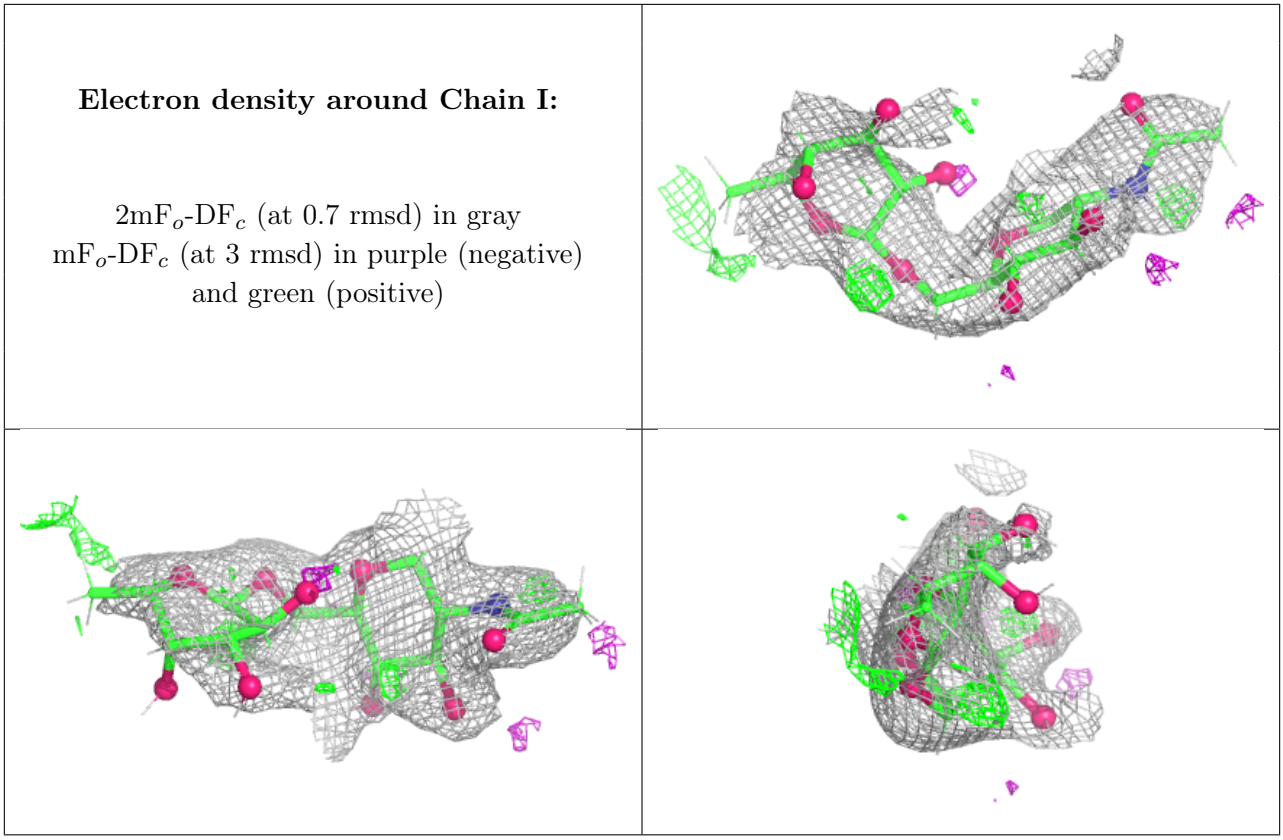
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain H:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	EDO	A	718	4/4	0.62	0.20	52,63,68,77	0
15	NAG	B	701	14/15	0.70	0.17	66,78,93,94	28
10	BO3	B	711	4/4	0.80	0.12	46,55,66,66	7
8	EDO	B	713	4/4	0.80	0.17	66,80,84,86	0
8	EDO	A	712	4/4	0.81	0.14	52,63,66,70	0
11	PGE	A	720[A]	10/10	0.83	0.15	28,37,44,45	24
11	PGE	A	720[B]	10/10	0.83	0.15	29,37,44,44	24
10	BO3	A	716	4/4	0.83	0.13	40,42,50,53	7
7	XPE	A	710	31/31	0.86	0.14	39,55,67,74	0
10	BO3	B	710	4/4	0.86	0.15	36,42,49,52	7
10	BO3	A	721	4/4	0.87	0.20	45,54,65,73	0
9	PEG	A	717	7/7	0.87	0.14	46,56,61,66	17
8	EDO	B	707	4/4	0.89	0.12	54,65,70,75	0
8	EDO	A	719	4/4	0.89	0.09	44,53,60,61	10

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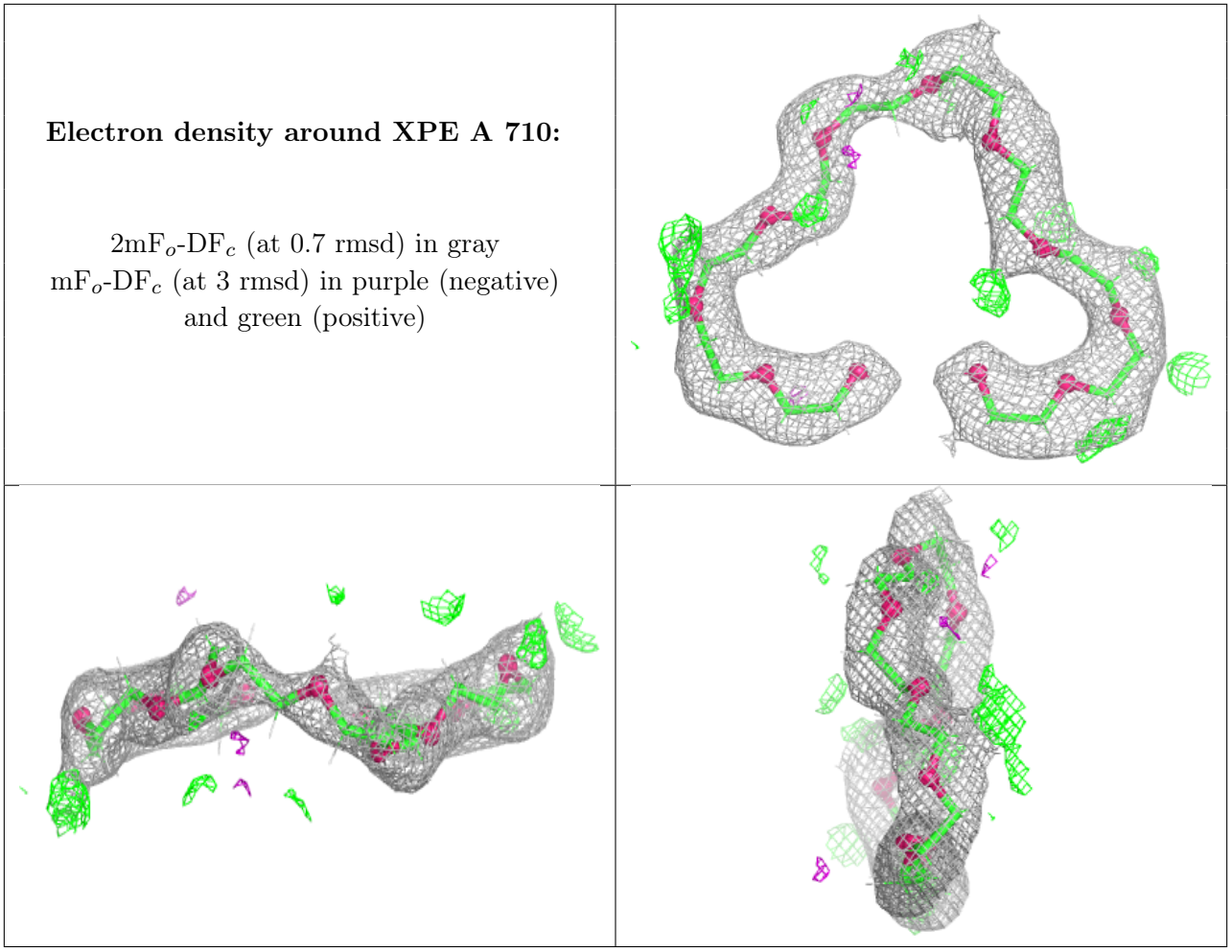
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	BO3	B	712	4/4	0.90	0.08	50,55,66,67	0
9	PEG	B	708	7/7	0.91	0.11	31,39,46,47	17
9	PEG	B	709	7/7	0.91	0.12	44,53,59,59	17
8	EDO	A	711	4/4	0.92	0.10	51,61,64,66	0
10	BO3	A	714	4/4	0.92	0.10	37,43,51,54	7
9	PEG	A	713	7/7	0.93	0.09	44,53,62,71	0
10	BO3	A	715	4/4	0.93	0.09	30,33,39,40	7
13	CL	B	716	1/1	0.94	0.14	44,44,44,44	0
14	MG	B	717	1/1	0.96	0.10	47,47,47,47	0
14	MG	A	725	1/1	0.96	0.07	38,38,38,38	1
12	ZN	B	714	1/1	0.98	0.03	29,29,29,29	1
13	CL	B	715	1/1	0.98	0.06	32,32,32,32	0
12	ZN	A	722	1/1	0.99	0.02	30,30,30,30	1
13	CL	A	724	1/1	1.00	0.07	36,36,36,36	0
13	CL	A	723	1/1	1.00	0.02	25,25,25,25	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around XPE A 710:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.